

Macroscopic description of microscopically strongly inhomogeneous systems

A mathematical basis for the synthesis of higher gradients metamaterials

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Abstract

We consider the time evolution of a one dimensional n -gradient continuum. Our aim is to construct and analyze discrete approximations in terms of physically realizable mechanical systems, called microscopic because they are living on a smaller space scale. We validate our construction by proving a convergence theorem of the microscopic system to the given continuum, as the scale parameter goes to zero.

1 Introduction

Continua with exotic behaviors are acquiring an increasing attention for their interest in technological applications (see e.g. [11, 26, 19, 1, 24, 29] and references therein). In this paper we address what, in a sense, is an inverse problem: given a continuum model we seek for those mechanical systems which, at a certain length scale, behave as specified by the chosen continuum model. The aim is to understand the microscopic properties of such systems to obtain information on how to realize (synthesize) them, at least in principle.

To be more precise, we are interested in a metamaterial which, roughly speaking, is an array of elementary individuals, much smaller than the typical macroscopic size, arranged in periodic structures and exhibiting unusual macroscopic behavior.

In our mathematical analysis we want to consider such a continuous system as described by a partial differential equation generated by a Lagrangian which summarizes all the macroscopic properties we may desire. Then we discretize this system and manage to identify such a discretization as a real conservative mechanical model. In other words we start from a macroscopic behavior and describe one possible microscopic interaction which realizes it at a macroscopic level. Finally we give a mathematical foundation to this procedure by proving a convergence result.

From a mathematical point of view, we underline once more that this is an inverse problem, compared to the one (largely unsolved) formulated by D. Hilbert in his famous speech in 1900 at ICM in Paris (see [15]) in which he encouraged to prove rigorously the transition from particle systems to fluid dynamics (Hilbert's 6-th problem). However it is worth to stress that we are working in the framework of continuum

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mechanics, but our microscopic elements, even if small in macro unities, are large compared with molecular scales.

We conclude this introduction by spending some more words on metamaterials, collocating them in the framework of generalized continua, with a particular emphasis to the pioneering work of G. Piola (see [9, 25, 2]).

The rest of the paper is organized as follows. In Section 2 we introduce continuous and discrete Lagrangians and discuss the identification problem, namely we specify the mechanical systems outlined by the discretization procedure. In Section 3 we formulate and solve the associated convergence problem.

We remark that our work concerns one-dimensional systems only. This is of course a severe limitation, but, on the other hand, it is a natural setting to start with.

1.1 Mechanical metamaterials

By suitably rephrasing Engheta and Ziolkowski [11] and Zouhdi et al. [29], metamaterials are materials which are first theoretically conceived and then engineered to have properties very unlikely to be found in nature.

They are obtained by suitably assembling multiple individual elements constructed with already available microscopic materials, but usually arranged in (quasi-)periodic sub-structures. Indeed the properties of metamaterials do not depend only on those of their component materials, but also on the topology of their connections and the nature of their mutual interaction forces. In literature it is currently specified a particular class of metamaterials, so called mechanical metamaterials, those in which the particular properties which are “designed” for the newly synthesized material are purely mechanical. The present paper deals exactly with such a class.

We explicitly remark here that in the present paper we use the adjective “microscopic” or “micro-” meaning all those length scales which are (much) smaller than the scale at which continuum mechanics is applicable. In particular we do not attach any value in SI units to each considered length scale.

The particular shape, geometry, size, orientation and arrangement of the elementary individual elements can affect, for instance, the propagation of waves of light or sound in a not-already-observed manner. In this way one can create material properties which cannot be found in conventional materials.

Particularly promising are those micro-structures which present high-contrast in microscopic properties. These structures, once homogenized, have shown to produce generalized continua (see e.g. [5, 1, 26]). These micro-structures, although remaining quasi-periodical, are conceived so that some of the physical properties which are characterizing their behavior are diverging when the size of the representative elementary volume tends to zero, while simultaneously some others are vanishing in this limit.

To give a hint of the possible applications of newly designed metamaterials we list here some among the papers which are more relevant to our results, especially in the perspective of their extension to 2D and 3D systems. In [18] it is shown how to synthesize a composite medium exhibiting negative effective bulk modulus, negative effective mass density (see also [5]), or both properties. In [16] materials with negative Poisson’s ratio (auxetics) was designed, and they were fabricated in 1999 (see Xu et al.[28]). One of the most famous examples of such materials is the Goretex whose negative Poisson ratio opened unexpected possibility to e.g. vascular surgery.

The damping effects can be also suitably designed using special selection of the material microstructure as reported in [3, 4], or the acoustic and optical effects as negative refraction, lensing and cloaking [6, 21].

All described materials can be modeled at a micro-level as finite dimensional Lagrangian systems and their effective properties were all obtained via a kind of homogenization procedure.

1.2 Generalized Continua

In the first half of XIX century the design of structures became an intellectual activity based on the rigorous application of predictive mathematical models. These models were formulated by means of a

precise postulation process and originated a series of problems or exercises directly motivated by the engineering applications, which were solved by means of the use of the then newly developed techniques of mathematical analysis.

The model describing the mechanical behaviour of materials introduced by Cauchy - although very accurate for a large class of phenomena - cannot be applied to all materials in every physical condition.

More general models were formulated by Gabrio Piola in the same years, but only recently they were considered in engineering for applications.

In some formulations of continuum mechanics, the possibility of the dependence of deformation energy on higher gradients of displacement, is rejected, due to an apparent (see [7]) incompatibility with the second principle of thermodynamics ([10],[14]). On the other hand, physicists, for instance Landau [17], always considered this dependence as admissible, as they are accustomed to base the postulation of physical theories on the principle of least action or on the principle of virtual works, which is exactly the same starting point of G. Piola [25].

Actually, when introducing Piola continua, the true conceptual frame settled by Cauchy, Navier and Poisson is to be drastically modified. The concept of stress becomes secondary and the main role is played by deformation measures together with action and dissipation functionals. The Euler-Lagrange equation obtained in this more encompassing modeling process cannot be anymore regarded to coincide with the balance of force unless one generalizes the concept of force. This can be done by introducing generalized actions as the dual quantities in the work of the gradients of displacements (see e.g. [13, 20, 22, 27, 12, 8, 23]).

Actually the same concept of contact interaction has to be completely modified, and the crucial point of determining the correct boundary conditions which can be assigned in generalized continua theory has been addressed only very recently (see e.g. [8]), following the original ideas by Piola [25].

2 Microscopic and Macroscopic descriptions

In what follows we will consider two length scales l and L with $l \ll L$. We will call microscopic or micro the description at the length scale l , while macroscopic or macro will be the attribute relative to the description which is suitable at the length scale L .

We assume that the most suitable micro-description at micro-scale is “discrete” i.e. based on the model “material particle” (as done by Poisson, Navier and -in some works- by Piola), while the description which has to be used at the macro-level is that of a continuum, as introduced e.g. by Lagrange, Cauchy or again Piola.

Remark however that we will not limit our attention to systems which verify the assumptions put forward by Cauchy and Navier. We will consider, actually, those continua which have been considered by Piola (and then by many others, including Toupin, Green, Rivlin and Mindlin) i.e. so called higher gradient continua.

To quantify the above considerations we will introduce, in the sequel, a small parameter $\varepsilon > 0$ indicating the ratio between typical micro and macro scales, possibly to be sent to zero to outline a suitable asymptotic behavior.

2.1 The basic macroscopic continuous model

Let $I = (0, L) \subset \mathbb{R}$ be a finite interval assumed as reference configuration of the considered one-dimensional continuum. We label each element of the continuum with the coordinate $x \in I$ of its placement in the reference configuration. The actual configuration of the continuum is described by the displacement field $u = u(x, t)$ which represents the horizontal displacement at time t of the element x from its position in the reference configuration.

Fixed an integer $n \geq 1$, for such a system we introduce the Lagrangian

$$\mathcal{L}(u, \dot{u}) = \frac{1}{2} \int_I |\dot{u}(x)|^2 - \int_I \Phi(u(x), Du(x), \dots, D^n u(x)). \quad (2.1)$$

Here, $D^k u$ is the k -th x -derivative of u and

$$\mathbb{R}^{n+1} \ni \underline{\xi} = (\xi_0, \dots, \xi_n) \mapsto \Phi(\underline{\xi}) \in \mathbb{R} \quad (2.2)$$

is a function whose properties will be specified later on.

Note that $\Phi(u, Du, \dots, D^n u)$ is the potential energy density corresponding to the displacement u and describes the constitutive properties of the medium under investigation.

The action on the time interval $(0, T)$ is consequently defined as

$$\mathcal{A} = \int_0^T \mathcal{L}(u(\cdot, t), \dot{u}(\cdot, t)), \quad (2.3)$$

where $\dot{u}(x, t) = \partial_t u(x, t)$ is the time derivative.

To deduce the Euler-Lagrange equations from the stationary action principle, we have first to specify the kinematic boundary condition for our problem. In the sequel we shall assume either

- periodic boundary conditions. Namely the reference configuration is \mathcal{C} , a circle of radius $\frac{L}{2\pi}$ (the points 0 and L are identified),
- or
- Dirichlet boundary conditions. Namely u and its first $n - 1$ derivatives vanish at 0 and L .

With above boundary conditions no boundary terms appear when performing the integrations by parts needed to obtain the equation of the motion (2.4) below.

Note also that the maximal order of the spatial derivatives appearing in the equation of motion (2.4) is $2n$.

The equation of motion, as a consequence of the stationary action principle and the boundary conditions, is (with $D^0 u = u$)

$$\ddot{u} = - \sum_{\alpha=0}^n (-1)^\alpha D^\alpha \partial_{\xi_\alpha} \Phi(u, Du, \dots, D^n u). \quad (2.4)$$

We could also include, in the present context, a given external potential with a very minor effort. We avoid to do so for notational simplicity.

Now we specify Φ by assuming that

$$\Phi(\underline{\xi}) = \frac{1}{2} (\underline{\xi}, Q \underline{\xi}) + R(\underline{\xi}) \quad (2.5)$$

i.e. the quadratic part of Φ is a quadratic form in terms of the displacement and its derivatives, contained in the vector $\underline{\xi}$. $Q = \{Q_{\alpha,\beta}\}_{\alpha,\beta=0}^n$ is a symmetric (without loss of generality) constant matrix with $Q_{n,n} \neq 0$.

On the non-linear part R we shall do suitable assumptions later on. We start by requiring that

$$R(\underline{0}) = 0, \quad R(\underline{\xi}) = O(|\underline{\xi}|^3), \quad (2.6)$$

namely the quadratic part of the interaction is fully expressed by the matrix Q .

The fact that Φ is not depending explicitly on x is consequence of the macroscopic homogeneity of the continuum (although it may be strongly inhomogeneous at microscopic scales). This implies that Q is constant.

As a first step we show that, in contrast with the fairly generality of the model, the quadratic part can be considerably simplified. Indeed, symmetrizing, integrating by parts and using the periodic or Dirichlet boundary conditions, we get:

$$\begin{aligned}
\mathcal{U} &\doteq \frac{1}{2} \sum_{\alpha, \beta=0}^n Q_{\alpha, \beta} \int_I D^\alpha u D^\beta u \\
&= \frac{1}{4} \sum_{\gamma=0}^{2n} \sum_{\substack{\alpha, \beta \geq 0: \\ \alpha + \beta = \gamma}} Q_{\alpha, \beta} \int_I u D^\gamma u [(-1)^\alpha + (-1)^\beta] \\
&= \frac{1}{4} \sum_{\gamma=0}^n \sum_{\substack{\alpha, \beta \geq 0: \\ \alpha + \beta = 2\gamma}} Q_{\alpha, \beta} [(-1)^\alpha + (-1)^\beta] (-1)^\gamma \int_I |D^\gamma u|^2 \\
&= \frac{1}{2} \sum_{\gamma=0}^n A_\gamma \int_I |D^\gamma u|^2,
\end{aligned} \tag{2.7}$$

where

$$A_\gamma = \frac{1}{2} \sum_{\substack{\alpha, \beta \geq 0: \\ \alpha + \beta = 2\gamma}} Q_{\alpha, \beta} [(-1)^\alpha + (-1)^\beta] (-1)^\gamma. \tag{2.8}$$

Note that in the first step in (2.7) we have used the symmetry of $Q_{\alpha, \beta}$ and in the second step we used that $(-1)^\alpha + (-1)^\beta = 0$ if $\alpha + \beta$ is odd. In the third step we have again integrated by parts.

As a consequence of this analysis, without loss of generality, we can assume Φ of the form

$$\Phi = \frac{1}{2} \sum_{\alpha=0}^n A_\alpha |\xi_\alpha|^2 + R(\underline{\xi}), \tag{2.9}$$

with $A_n \neq 0$ and the equations of motion are

$$\ddot{u} = - \sum_{\alpha=0}^n (-1)^\alpha A_\alpha \Delta^\alpha u - \sum_{\alpha=0}^n (-1)^\alpha D^\alpha \partial_{\xi_\alpha} \mathbb{R}(u, Du, \dots, D^n u), \tag{2.10}$$

where $\Delta = D^2$ denotes the Laplacian. Note that in the linear part only even derivatives are allowed.

2.2 Formal discretization

In view of the construction of the mechanical (microscopic) system with a finite number of degrees of freedom, we introduce a finite lattice of mesh ε in I . The lattice points are $\{0, \varepsilon, 2\varepsilon, \dots, k\varepsilon, \dots, N\varepsilon\}$ with the obvious condition $N\varepsilon = L$. When considering periodic boundary conditions we clearly identify 0 with εN .

We associate to each lattice point a *microscopic* particle of unitary mass labelled by the index $i \in \{0, \dots, N\}$ and denote by u_i the displacement of the particle i from the reference position $i\varepsilon$. The array $u_\varepsilon = \{u_i\}_{i=0}^N$ is the discretized displacement field.

The discretized Lagrangian takes the form

$$\mathcal{L}_\varepsilon(u_\varepsilon, \dot{u}_\varepsilon) = \frac{1}{2} \sum_{i=0}^N \varepsilon \dot{u}_i^2 - U(u_\varepsilon), \tag{2.11}$$

where

$$U(u_\varepsilon) = \sum_{i=0}^N \varepsilon \left[\frac{1}{2} \sum_{\alpha=0}^n A_\alpha |(D_\varepsilon^\alpha u_\varepsilon)_i|^2 + R((\underline{D}_\varepsilon u_\varepsilon)_i) \right], \tag{2.12}$$

where $(\underline{D_\varepsilon u_\varepsilon})_i = \{(D_\varepsilon^\alpha u_\varepsilon)_i\}_{\alpha=0}^n$,

$$D_\varepsilon^\alpha u = \begin{cases} \Delta_\varepsilon^{\frac{\alpha}{2}} u_\varepsilon, & \alpha \text{ even}, \\ D_\varepsilon^+ \Delta_\varepsilon^{\frac{\alpha-1}{2}} u_\varepsilon, & \alpha \text{ odd}. \end{cases} \quad (2.13)$$

Here D_ε^+ and D_ε^- , defined as

$$(D^+ u_\varepsilon)_i = \frac{u_{i+1} - u_i}{\varepsilon}, \quad (D^- u_\varepsilon)_i = \frac{u_i - u_{i-1}}{\varepsilon}, \quad (2.14)$$

are the right and left discrete derivatives respectively and Δ_ε , defined by

$$(\Delta_\varepsilon u_\varepsilon)_i = (D_\varepsilon^+ D_\varepsilon^- u_\varepsilon)_i = (D_\varepsilon^- D_\varepsilon^+ u_\varepsilon)_i = \frac{1}{\varepsilon^2} (u_{i+1} + u_{i-1} - 2u_i). \quad (2.15)$$

is the discrete Laplacian.

To complete the above definitions we need to define the discrete derivatives at the boundary. For periodic boundary conditions it is enough to use the following convention: for any $k \in \mathbb{Z}$,

$$u_{N+k} = u_k. \quad (2.16)$$

For Dirichlet boundary condition, we have to think of the first and last n particles frozen in their reference position. Hence we assume the constraints

$$u_i = 0, \quad i \in \{0, \dots, n-1\} \cup \{N-n+1, \dots, N\}. \quad (2.17)$$

The equations of motion are

$$\ddot{u}_i = F_i, \quad F_i = -\frac{\partial U}{\partial u_i}, \quad (2.18)$$

with the index i running from 1 to N in the periodic case and on the set of i 's for which u_i is not constrained in the Dirichlet case. We notice that the choice of the right derivative (as well as any other possible discretization) is arbitrary. The only restriction that we have is the mechanical realizability (in principle) of this system. We are going to discuss this point in the next subsection.

We finally remark that F_i depends on u_j , with $|i-j| \leq n$. However this is an almost local contribution because n is fixed and those u_j 's influencing u_i are at macroscopic distance $O(\varepsilon)$.

2.3 Realizable syntheses

The aim of this subsection is to show that, at least in the simplest case of linear forces, the above introduced discrete system corresponds to a system of particles interacting via two-body forces of range not larger than n . Therefore, it can be realized by suitably assembling mechanical elements.

Let us consider the linear system introduced in (2.4) with $R = 0$ and its discrete counterpart (2.18). It can be checked that

$$F_i = -\sum_{k=0}^n (-1)^k A_k \Delta_\varepsilon^k u_\varepsilon(x_i). \quad (2.19)$$

Therefore, the force acting on the particle i is expressed as a linear combination of discrete derivatives up to the order $2n$.

We want to show that F_i can be interpreted as the result of the action of a system of linear pairwise forces with suitable range. More precisely, we want to find ε -dependent coefficients $k_{i,j}$ such that

$$F_i = \sum_j k_{i,j} (u_j - u_i) \quad (2.20)$$

and hence

$$U(u_1, \dots, u_N) = \frac{1}{2} \sum_{i,j=1}^N k_{i,j} (u_i - u_j)^2. \quad (2.21)$$

We prove below that for any p ,

$$(\Delta^p u)_i = \sum_j K_{i,j}^p (u_j - u_i), \quad (2.22)$$

with $K_{i,j}^p$ other suitable constants. Once (2.22) is proved, we can conclude that (2.20) holds with

$$k_{i,j} = \sum_{p=0}^n (-1)^p A_p K_{i,j}^p. \quad (2.23)$$

Note that the constants $k_{i,j}$ are not necessarily all positive even if the A_α are all positive.

The constants $K_{i,j}^p$ are given by the recursive equation (2.28) below. It implies that, for any p , $K_{i,j}^p$ vanishes for $|i - j| > p$, thus $k_{i,j} = 0$ if $|i - j| > n$. Moreover, in the periodic case $K_{i,j}^p$ depends only on the difference $i - j$ and is symmetric in the exchange $i \leftrightarrow j$ and hence the *action-reaction* principle is satisfied.

We prove (2.22) by recurrence.

For $p = 1$, we have

$$(\Delta_\varepsilon u)_i = \varepsilon^{-2} (u_{i+1} + u_{i-1} - 2u_i) = \varepsilon^{-2} (u_{i+1} - u_i) + \varepsilon^{-2} (u_{i-1} - u_i). \quad (2.24)$$

Thus (2.22) is verified with

$$K_{i,i+1}^1 = K_{i,i-1}^1 = \varepsilon^{-2} \quad \text{and} \quad K_{i,j}^1 = 0 \quad \text{otherwise.} \quad (2.25)$$

Suppose now that (2.22) is true for $p = \ell - 1$:

$$(\Delta_\varepsilon^{\ell-1} u)_i = \sum_j K_{i,j}^{\ell-1} [u_j - u_i].$$

Then,

$$\begin{aligned} (\Delta_\varepsilon^\ell u)_i &= (\Delta_\varepsilon^{\ell-1} \Delta_\varepsilon u)_i = \sum_j K_{i,j}^{\ell-1} [(\Delta_\varepsilon u)_j - (\Delta_\varepsilon u)_i] \\ &= \sum_j K_{i,j}^{\ell-1} [\varepsilon^{-2} (u_{j+1} - u_j) + \varepsilon^{-2} (u_{j-1} - u_j) - \varepsilon^{-2} (u_{i+1} - u_i) - \varepsilon^{-2} (u_{i-1} - u_i)] \\ &= \sum_j K_{i,j}^{\ell-1} [\varepsilon^{-2} (u_{j+1} - u_i) - \varepsilon^{-2} (u_j - u_i) + \varepsilon^{-2} (u_{j-1} - u_i) - \varepsilon^{-2} (u_j - u_i) \\ &\quad - \varepsilon^{-2} (u_{i+1} - u_i) - \varepsilon^{-2} (u_{i-1} - u_i)]. \end{aligned} \quad (2.26)$$

Using the change of index $j + 1 \rightarrow j$ in the first term and $j - 1 \rightarrow j$ in the second, we have

$$\begin{aligned} (\Delta_\varepsilon^\ell u)_i &= \sum_j K_{i,j-1}^{\ell-1} \varepsilon^{-2} (u_j - u_i) - K_{i,j}^{\ell-1} \varepsilon^{-2} (u_j - u_i) + K_{i,j+1}^{\ell-1} \varepsilon^{-2} (u_j - u_i) \\ &\quad - \varepsilon^{-2} K_{i,j}^{\ell-1} (u_j - u_i) - \varepsilon^{-2} K_{i,j}^{\ell-1} (u_{i+1} - u_i) - \varepsilon^{-2} K_{i,j}^{\ell-1} (u_{i-1} - u_i)]. \end{aligned} \quad (2.27)$$

Thus, (2.22) is verified with the following recursive definition of $K_{i,j}^\ell$:

$$K_{i,j}^\ell = \varepsilon^{-2} \left[K_{i,j-1}^{\ell-1} + K_{i,j+1}^{\ell-1} - 2K_{i,j}^{\ell-1} - (\delta_{i+1,j} + \delta_{i-1,j}) \sum_{j'} K_{i,j'}^{\ell-1} \right], \quad (2.28)$$

for $\ell > 1$ and $K_{i,j}^1$ given by (2.25).

Equations (2.28) and (2.23) solve definitely the posed problem of identifying the topology of the microstructure connections, since they provide the coefficients $k_{i,j}$ only in terms of the coefficients A_p that characterize the continuous formulation of the macroscopic description of the elastic problem.

3 A rigorous result of convergence

In this section we prove a convergence result of the discrete model introduced in the previous section to the prescribed continuous systems in the limit as the scale parameter goes to 0. We show the convergence of the solution of the discrete system to the continuous one in the energy norm of the system. To clarify the argument without the use of cumbersome notation, we present first a paradigmatic case for which we discuss both periodic and Dirichlet boundary conditions. The more general case is considered in Subsection 3.2 where we give the convergence proof only in the periodic case although the argument can be straightforwardly extended to the Dirichlet boundary conditions as well.

For the reader convenience we rewrite the Lagrangian we are going to consider in this Section, namely

$$\mathcal{L}(u, \dot{u}) = \frac{1}{2} \int_I dx |\dot{u}(x, t)|^2 - \frac{1}{2} \sum_{\alpha=1}^n \int_I dx |D^\alpha u|^2(x, t)^2 - \int_I R(u, Du, D^2u \dots). \quad (3.1)$$

As we shall see later on, we will consider only nonlinear terms R depending on u and the first derivative only.

3.1 The Δ^2 case - dynamic Euler-Bernoulli beam: “Elastica”

3.1.1 Periodic boundary conditions

We consider the Lagrangian (3.1) with $A_0 = A_1 = 0$ and $A_2 = 1$. Moreover we focus on the linear case $R = 0$. Thus we have the following linear initial value problem in the circle, \mathcal{C} :

$$\ddot{u} = -\frac{\partial^4 u}{\partial x^4} := -\Delta^2 u, \quad (3.2)$$

$$u(x, 0) = u_0(x), \quad \dot{u}(x, 0) = v_0(x). \quad (3.3)$$

It is well known that there exists a unique classical solution as the initial data are assumed sufficiently smooth.

More precisely we assume that

$$u_0 \in H^s, \quad v_0 \in H^r \quad \text{with} \quad s \geq 6, r \geq 4, \quad (3.4)$$

where H^s denotes the Sobolev space endowed with norm

$$\|u\|_{H^s} = \sum_{\ell=0}^s \|D^\ell u\|_2^2,$$

and $\|\cdot\|_p$ is the $L^p(\mathcal{C})$ -norm.

In this way, by using the well known energy method, we can prove the propagation (in time) of the H^s regularity for u and \dot{u} , yielding, in particular, $u \in C^5(\mathcal{C})$ (as consequence of the obvious inequality $\|u\|_\infty \leq C\|u\|_{H^1}$).

Next we consider the mechanical system of N particles, with coordinates u_i , $i = 1, \dots, N$, whose Lagrangian is given by (2.11) again with $A_0 = A_1 = 0$, $A_2 = 1$ and $R = 0$. The equation of motion are explicitly

$$\ddot{u}_i = \frac{1}{\varepsilon^4} (-u_{i+2} + 4u_{i+1} - 6u_i - u_{i-2} + 4u_{i-1}) \quad i = 1 \dots N, \quad (3.5)$$

with the convention $u_{N+k} = u_k$ for any $k \in \mathbb{Z}$.

We want to compare the solutions of (3.2) with the corresponding ones of (3.5). To do this we first set

$$u_\varepsilon(x, t) = u_i(t) \quad \text{if} \quad x \in [i\varepsilon, (i+1)\varepsilon), \quad i \in \{1, \dots, N\}. \quad (3.6)$$

In other words we introduce a function u_ε which is the step, left continuous, function (constant in the lattice interval) taking the value of the nearest left point of the lattice. Problem (3.5) is rephrased accordingly:

$$\ddot{u}_\varepsilon(x, t) = -\Delta_\varepsilon^2 u_\varepsilon(x, t) \quad x \in \mathcal{C}, \quad (3.7)$$

where

$$\Delta_\varepsilon u(x) = D_\varepsilon^+ D_\varepsilon^- u(x) \quad (3.8)$$

$$D^\pm u(x) = \pm \frac{1}{\varepsilon} (u(x \pm \varepsilon) - u(x)). \quad (3.9)$$

Notice that the Lagrangian (2.11), with $A_0 = A_1 = 0$, $A_2 = 1$ and $R = 0$, has the following continuous representation:

$$\mathcal{L}(u_\varepsilon, \dot{u}_\varepsilon) = \int_{\mathcal{C}} dx \left[\frac{1}{2} \dot{u}_\varepsilon(x, t)^2 - \frac{1}{2} (\Delta_\varepsilon u_\varepsilon(x, t))^2 \right]. \quad (3.10)$$

We suppose that, at the initial time, $u_\varepsilon, \dot{u}_\varepsilon$ are approximating u, \dot{u} in the sense that

$$u_\varepsilon(x, 0) = u_0(i\varepsilon), \quad \dot{u}_\varepsilon(x, 0) = v_0(i\varepsilon) \quad \text{if } x \in [i\varepsilon, (i+1)\varepsilon). \quad (3.11)$$

Note that, by the conservation of the energy, we have

$$\mathcal{E}[u(t)] := \frac{1}{2} \int_{\mathcal{C}} dx \left[|\dot{u}(t)|^2 + |\Delta u(t)|^2 \right] = \mathcal{E}[u(0)], \quad (3.12)$$

as well as

$$\mathcal{E}_\varepsilon[u_\varepsilon(t)] := \frac{1}{2} \int_{\mathcal{C}} dx \left[|\dot{u}_\varepsilon(t)|^2 + |\Delta_\varepsilon u_\varepsilon(t)|^2 \right] = \mathcal{E}_\varepsilon[u_\varepsilon(0)]. \quad (3.13)$$

Next we introduce the following function which controls the deviation of u_ε from u :

$$W_\varepsilon(t) = \frac{1}{2} \int_{\mathcal{C}} dx \left[(u_\varepsilon(x, t) - u(x, t))^2 + (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))^2 + [\Delta_\varepsilon(u_\varepsilon(x, t) - u(x, t))]^2 \right]. \quad (3.14)$$

Computing the time derivative and using the equation of motion we get

$$\begin{aligned} \dot{W}_\varepsilon(t) = & \int_{\mathcal{C}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))(u_\varepsilon(x, t) - u(x, t) + \ddot{u}_\varepsilon(x, t) - \ddot{u}(x, t)) + \\ & \int_{\mathcal{C}} dx \Delta_\varepsilon(u_\varepsilon(x, t) - u(x, t)) \Delta_\varepsilon(\dot{u}_\varepsilon(x, t) - \dot{u}(x, t)) = \\ & + \int_{\mathcal{C}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))(u_\varepsilon(x, t) - u(x, t)) \\ & - \int_{\mathcal{C}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t)) \Delta_\varepsilon^2(u_\varepsilon(x, t) - u(x, t)) \\ & + \int_{\mathcal{C}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t)) (\Delta^2 u(x, t) - \Delta_\varepsilon^2 u(x, t)) \\ & + \int_{\mathcal{C}} dx \Delta_\varepsilon(u_\varepsilon(x, t) - u(x, t)) \Delta_\varepsilon(\dot{u}_\varepsilon(x, t) - \dot{u}(x, t)). \end{aligned} \quad (3.15)$$

Now consider the following discrete integration by parts formula, namely

$$\int_{\mathcal{C}} f(x) D_\varepsilon^\pm g(x) = - \int_{\mathcal{C}} D_\varepsilon^\mp f(x) g(x) \quad (3.16)$$

valid for any couple of bounded functions f and g .

If we apply the above formula twice we conclude that the second and fourth terms in (3.15) cancel each other. On the other hand the first term is bounded by

$$\frac{1}{2} \int_{\mathcal{C}} dx |\dot{u} - \dot{u}_\varepsilon|^2 + |u - u_\varepsilon|^2 \leq W.$$

The third term is bounded by

$$\frac{1}{2} \int_{\mathcal{C}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))^2 + \frac{1}{2} \int_{\mathcal{C}} |(\Delta^2 - \Delta_\varepsilon^2)u(x, t)|^2.$$

Now the first term of the expression above is bounded by W . The second one, by the regularity of u and its derivatives up to the fifth order, is bounded, uniformly in $x \in \mathcal{C}$ and in t in any bounded interval, by a constant ω_ε vanishing as $\varepsilon \rightarrow 0$. Here and in the rest of the paper $\omega_\varepsilon \in \mathbb{R}$ denotes such a generic infinitesimal constant.

In conclusion, by the Gronwall lemma,

$$W_\varepsilon(t) \leq W_\varepsilon(0)e^{2t} + \omega_\varepsilon t e^{2t} \quad (3.17)$$

so that $W_\varepsilon(t)$ is vanishing, because $W_\varepsilon(0) \rightarrow 0$ by the regularity of u and the assumptions on initial data.

We summarize above discussion in the following

Theorem 3.1. *Suppose that u_0 and v_0 satisfy (3.4). Let $u(t)$ be the solution to (3.2) and $u_\varepsilon(t)$ be the step function defined by (3.6) with $u_i(t)$, $i = 1, \dots, N$, solutions to (3.5) with initial data $u_i(0) = u_0(i\varepsilon)$ and $\dot{u}_i(0) = v_0(i\varepsilon)$. Then, for any $t \in \mathbb{R}$,*

$$\lim_{\varepsilon \rightarrow 0} W_\varepsilon(t) = 0.$$

3.1.2 Dirichlet boundary conditions

For the Dirichlet boundary conditions we replace the circle \mathcal{C} with the interval $I = [0, L]$. The equation (3.2) is well posed with the boundary conditions

$$u(0, t) = u'(0, t) = u(L, t) = u'(L, t) = 0. \quad (3.18)$$

Remark: Several other boundary conditions may have an interest in engineering application and a physical meaning. For instance the conditions $u(0) = u''(0) = 0$, $u(L) = u''(L) = 0$, characterizes a beam with pivots applied at its endpoints, while the conditions which we considered here are relative to clamped-clamped beams. We do not consider in this paper the other possible boundary conditions, as the focus of this paper is different.

Again, by using the energy method, we can construct solution with H^s regularity, by assuming

$$u_0 \in H_0^2 \cap H^s, \quad v_0 \in H_0^2 \cap H^r \quad \text{with} \quad s \geq 6, r \geq 4. \quad (3.19)$$

Here H_0^2 (introduced to take into account the boundary conditions) is defined as the space of the H^2 functions vanishing in 0 and L , together with their first derivative.

The corresponding discrete system is constituted by $N-3$ particles with coordinates u_i , $i = 2, \dots, N-2$ and

$$u_0 = u_1 = u_{N-1} = u_N = 0 \quad (3.20)$$

are the constraints corresponding to the Dirichlet boundary conditions.

With this position, the explicit equations of motion are

$$\ddot{u}_i = \frac{1}{\varepsilon^4}(-u_{i+2} + 4u_{i+1} - 6u_i - u_{i-2} + 4u_{i-1}) \quad i = 2 \dots N-2, \quad (3.21)$$

As before we introduce the left continuous step function

$$u_\varepsilon(x, t) = u_i(t) \quad \text{if } x \in [i\varepsilon, (i+1)\varepsilon), \quad i \in \{0, \dots, N-1\}, \quad (3.22)$$

but we find convenient to think of it as a function on \mathbb{R} extended with value 0 outside I . Then (3.21) can be rewritten similarly to (3.7) as

$$\ddot{u}_\varepsilon(x, t) = -\Delta_\varepsilon^2 u_\varepsilon(x, t) \quad x \in I_\varepsilon = (2\varepsilon, L - \varepsilon). \quad (3.23)$$

Note that the values of u_i are frozen for $i = 0, 1, N-1, N$, so that $u_\varepsilon = 0$ in $I_\varepsilon^c = I - I_\varepsilon$. We also think of the solution u of the continuous equation as extended with value 0 outside of I

Next we introduce the function $W_\varepsilon(t)$ as

$$W_\varepsilon(t) = \frac{1}{2} \int_{\mathbb{R}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))^2 + \frac{1}{2} \int_{\mathbb{R}} dx [\Delta_\varepsilon(u_\varepsilon(x, t) - u(x, t))]^2. \quad (3.24)$$

Note that this function differs from the one defined by integrating on I instead of \mathbb{R} because Δ_ε is non-local. It is actually larger and hence provides a stronger control of the convergence. Now we compute again the time derivative of W , as before and we get

$$\dot{W}_\varepsilon(t) = \int_{\mathbb{R}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))(\ddot{u}_\varepsilon(x, t) - \ddot{u}(x, t)) + \int_{\mathbb{R}} dx \Delta_\varepsilon(u_\varepsilon(x, t) - u(x, t))\Delta_\varepsilon(\dot{u}_\varepsilon(x, t) - \dot{u}(x, t)). \quad (3.25)$$

By using twice the discrete integration by parts formula

$$\int_{\mathbb{R}} dx f D_\varepsilon^\pm g = - \int_{\mathbb{R}} g D_\varepsilon^\mp f,$$

valid of any couple of bounded compactly supported functions f and g , the second term becomes, as before

$$\int_{\mathbb{R}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))\Delta_\varepsilon^2(u_\varepsilon(x, t) - u(x, t)).$$

As for the the first term, we need to use the equations of motion (3.2) for u and (3.23) for u_ε . Note that the last ones hold only in I_ε . Thus, using that $\ddot{u}_\varepsilon = 0$ in $\mathbb{R} - I_\varepsilon$, the first term becomes

$$\begin{aligned} & - \int_{I_\varepsilon} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))(\Delta_\varepsilon^2 u_\varepsilon(x, t) - \Delta^2 u(x, t)) - \int_{\mathbb{R} - I_\varepsilon} (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))(-\Delta^2 u(x, t)) = \\ & - \int_{\mathbb{R}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))(\Delta_\varepsilon^2 u_\varepsilon(x, t) - \Delta^2 u(x, t)) + \int_{\mathbb{R} - I_\varepsilon} (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))\Delta_\varepsilon^2 u_\varepsilon(x, t). \end{aligned} \quad (3.26)$$

By adding and subtracting the term $\int_{\mathbb{R}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))(\Delta_\varepsilon^2 u_\varepsilon(x, t) - \Delta_\varepsilon^2 u(x, t))$ the above term becomes

$$\begin{aligned} & - \int_{\mathbb{R}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))(\Delta_\varepsilon^2 u_\varepsilon(x, t) - \Delta_\varepsilon^2 u(x, t)) - \int_{\mathbb{R}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))(\Delta_\varepsilon^2 u(x, t) - \Delta^2 u(x, t)) \\ & + \int_{\mathbb{R} - I_\varepsilon} (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))\Delta_\varepsilon^2 u_\varepsilon(x, t). \end{aligned} \quad (3.27)$$

Putting together all these terms we conclude that

$$\dot{W} = - \int_{\mathbb{R}} dx (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))(\Delta_\varepsilon^2 u(x, t) - \Delta^2 u(x, t)) + \int_{\mathbb{R} - I_\varepsilon} (\dot{u}_\varepsilon(x, t) - \dot{u}(x, t))\Delta_\varepsilon^2 u_\varepsilon(x, t) \quad (3.28)$$

The first term in the right hand side of (3.28) goes to 0 as in the periodic case, by the regularity u . The second term is the novelty of the Dirichlet case. In order to estimate it, note that $\dot{u}_\varepsilon = 0$ outside of I_ε , hence we need to estimate $\int_{\mathbb{R}-I_\varepsilon} \dot{u}(x, t) \Delta_\varepsilon^2 u_\varepsilon(x, t)$.

By the boundary conditions on u , ($u = 0$ and $u' = 0$ in 0 and L for any t), it results (by our assumptions $|\Delta \dot{u}(x, t)|$ is bounded)

$$|\dot{u}(x, t)| \leq \frac{1}{2} \sup_{x \in \mathcal{I}} |\Delta \dot{u}(x, t)| \varepsilon^2 \quad x \in I_\varepsilon^c. \quad (3.29)$$

Furthermore

$$\Delta_\varepsilon^2 u_\varepsilon(x) = \varepsilon^{-2} (\Delta_\varepsilon u_\varepsilon(x + \varepsilon) + \Delta_\varepsilon u_\varepsilon(x - \varepsilon) - 2\Delta_\varepsilon u_\varepsilon(x)).$$

Rewriting the total energy (3.13) in a more explicit form,

$$\mathcal{E}[u_\varepsilon] = \frac{1}{2} \sum_{i=2}^{N-2} \varepsilon |\dot{u}_\varepsilon(i\varepsilon)|^2 + \frac{1}{2} \sum_{i=1}^N \varepsilon |\Delta_\varepsilon u_\varepsilon(i\varepsilon)|^2, \quad (3.30)$$

we obtain, at any time and for any x in \mathcal{I}_ε ,

$$|\Delta_\varepsilon u_\varepsilon(x)| \leq \frac{\sqrt{2E_0}}{\sqrt{\varepsilon}}, \quad (3.31)$$

where $E_0 = \mathcal{E}(u(0))$ is the energy of the initial data. Hence

$$\sup_{x \in I} |\Delta_\varepsilon^2 u_\varepsilon(x)| \leq 4\sqrt{2E_0} \varepsilon^{-\frac{5}{2}}. \quad (3.32)$$

Combining (3.29) and (3.32) and using the fact that the integration is restricted to the set $I - I_\varepsilon$, whose measure is 4ε (remind that $\dot{u} = 0$ outside \mathcal{I}), we conclude that

$$\left| \int_{\mathbb{R}-I_\varepsilon} \dot{u}(x, t) \Delta_\varepsilon^2 u_\varepsilon(x, t) \right| \leq C\sqrt{\varepsilon}.$$

The rest of the argument proceeds as before and we conclude that $W_\varepsilon(t) \rightarrow 0$.

We summarize above discussion in the following

Theorem 3.2. *Suppose that u_0 and v_0 satisfy (3.19). Let $u(t)$ be the classical solution to (3.2) with boundary conditions (3.18) and initial values (3.3) and $u_\varepsilon(t)$ be the step function defined by (3.22) with $u_i(t)$, $i = 2, \dots, N-2$, solutions to (3.21) with initial data $u_i(0) = u_0(i\varepsilon)$ and $\dot{u}_i(0) = v_0(i\varepsilon)$. Then, for any $t \in \mathbb{R}$,*

$$\lim_{\varepsilon \rightarrow 0} W_\varepsilon(t) = 0.$$

3.2 A n -th gradient case

Now we extend the previous argument to the more general setup corresponding to the Lagrangian (3.1), restricting the discussion to the simpler case of periodic boundary conditions. The Dirichlet boundary conditions can be handled as in the previous subsection but we avoid here unnecessary complications.

We assume the following conditions:

1.

$$A_0 > 0, \quad A_n > 0, \quad A_\alpha \geq 0, \quad \alpha = 1, \dots, n-1 \quad (3.33)$$

2. We have already supposed that $R(\underline{0}) = 0$ and $R(\underline{\xi}) = O(|\underline{\xi}|^3)$. In addition we assume that, for $n = 1$, R depends only on u and, for $n \geq 2$, R depends only on u and Du . Moreover we assume $R \in C^{2n+2}(\mathbb{R}^2)$.

Remark 3.1: The positivity assumptions on the A_α 's with $\alpha = 1, \dots, n-1$, can be relaxed. In facts, let us define, for some $\varepsilon_0 > 0$,

$$\kappa = \sup_{\varepsilon \in (0, \varepsilon_0)} \sup_{u: \|D_\varepsilon u\|_2 \leq 1} \frac{\|u\|_2^2}{\|D_\varepsilon u\|_2^2}, \quad (3.34)$$

with the supremum on u taken on all u with 0 average. Then it is enough to assume

$$\sum_{\alpha=1: A_\alpha < 0}^{n-1} |A_\alpha| \kappa^{n-\alpha} \leq \frac{1}{2} A_n, \quad (3.35)$$

to make the argument of the proof still working. This remark allows us to consider, for instance, the case $\ddot{u} = (-\Delta^2 - \gamma\Delta)u$, with γ sufficiently small, excluded by (3.33).

Remark 3.2: The assumption on R concerning its dependence on u and Du only, is restrictive. We do not expect any surprise in assuming an explicit dependence on some higher derivatives. However, as we shall see in the course of the proof, more general assumptions would complicate the algebraic manipulations in dealing with the discrete derivatives in a consistent way.

As regards the initial data we assume

$$u_0 \in H^{2n+2}, \quad v_0 \in H^{n+2}, \quad (3.36)$$

and, as before, the H^s regularity is propagated. Clearly $u \in C^{2n+1}(\mathcal{C})$.

The explicit equation is

$$\ddot{u} + \sum_{\alpha=0}^n (-1)^\alpha A_\alpha \Delta^\alpha u + \partial_{\xi_0} R(u, Du) - D[\partial_{\xi_1} R(u, Du)] = 0. \quad (3.37)$$

Note that thanks to the energy conservation,

$$\mathcal{E}[u] = \int_{\mathcal{C}} dx \left[\frac{1}{2} \left\{ \dot{u}^2 + \sum_{\alpha=0}^n A_\alpha |D^\alpha u|^2 \right\} + R(u, Du) \right], \quad (3.38)$$

we get immediately an a priori bound on the L^2 norm of u , \dot{u} and $D^n u$:

$$\frac{1}{2} \int_{\mathcal{C}} dx \left[|\dot{u}|^2 + A_0 |u|^2 + A_n |D^n u|^2 \right] \leq \mathcal{E}[u(0)]. \quad (3.39)$$

Now we remind the discrete counterpart of the above setup, which corresponds to the discrete Lagrangian (2.11). Using the discontinuous function

$$u_\varepsilon(x, t) = u_i(t) \quad \text{if } x \in [i\varepsilon, (i+1)\varepsilon), \quad (3.40)$$

as in the previous section, the discrete Lagrangian can be written as

$$\mathcal{L}_\varepsilon = \int_{\mathcal{C}} dx \left[\frac{1}{2} |\dot{u}_\varepsilon(x, t)|^2 - \frac{1}{2} \sum_{\alpha=0}^n A_\alpha |D_\varepsilon^\alpha u_\varepsilon(x, t)|^2 - R(u_\varepsilon(x, t), D_\varepsilon^+ u_\varepsilon(x, t)) \right]. \quad (3.41)$$

We can write the associated equations of motion in terms of u_ε as

$$\ddot{u}_\varepsilon + \sum_{\alpha=0}^n (-1)^\alpha A_\alpha \Delta_\varepsilon^\alpha u_\varepsilon + \partial_{\xi_0} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon) - D_\varepsilon^- [\partial_{\xi_1} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon)] = 0. \quad (3.42)$$

Also for the discrete system the energy conservation holds. Thus we have that

$$\mathcal{E}_\varepsilon[u_\varepsilon] = \int_{\mathcal{C}} dx \left[\frac{1}{2} \left\{ \dot{u}_\varepsilon^2 + \sum_{\alpha=0}^n A_\alpha |D_\varepsilon^\alpha u|^2 \right\} + R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon) \right] \quad (3.43)$$

is conserved and hence, using that $R \geq 0$, we have the inequality

$$\frac{1}{2} \int_{\mathcal{C}} dx \left[|\dot{u}_\varepsilon|^2 + A_0 |u_\varepsilon|^2 + A_n |D_\varepsilon^n u_\varepsilon|^2 \right] \leq \mathcal{E}_\varepsilon[u_\varepsilon(0)]. \quad (3.44)$$

Since $A_0 > 0$ and $A_n > 0$, the existence, globally in time, for the solution to the discrete system follow from this bound.

We start by proving the convergence of the discrete system to the continuous one in the linear case, namely when $R = 0$,

$$\ddot{u} + \sum_{\alpha=0}^n (-1)^\alpha A_\alpha \Delta^\alpha u = 0. \quad (3.45)$$

Similarly, the discrete system becomes

$$\ddot{u}_\varepsilon + \sum_{\alpha=0}^n (-1)^\alpha A_\alpha \Delta_\varepsilon^\alpha u_\varepsilon = 0. \quad (3.46)$$

We introduce

$$W_\varepsilon(t) = \frac{1}{2} \int_{\mathcal{C}} dx \left\{ |u(x, t) - u_\varepsilon(x, t)|^2 + |\dot{u}(x, t) - \dot{u}_\varepsilon(x, t)|^2 \right\} + \int_{\mathcal{C}} dx \sum_{\alpha=0}^n A_\alpha |D_\varepsilon^\alpha [u(x, t) - u_\varepsilon(x, t)]|^2. \quad (3.47)$$

The time derivative of W is:

$$\begin{aligned} \frac{d}{dt} W_\varepsilon &= \int_{\mathcal{C}} dx \left\{ (\dot{u} - \dot{u}_\varepsilon)(u - u_\varepsilon + \ddot{u} - \ddot{u}_\varepsilon) + \sum_{\alpha=0}^n A_\alpha D_\varepsilon^\alpha (\dot{u} - \dot{u}_\varepsilon) D_\varepsilon^\alpha (u - u_\varepsilon) \right\} \\ &= \int_{\mathcal{C}} dx (\dot{u} - \dot{u}_\varepsilon) \left\{ (u - u_\varepsilon + \ddot{u} - \ddot{u}_\varepsilon) + \sum_{\alpha=0}^n (-1)^\alpha A_\alpha \Delta_\varepsilon^\alpha (u - u_\varepsilon) \right\} \\ &= \int_{\mathcal{C}} dx (\dot{u} - \dot{u}_\varepsilon) \left\{ (u - u_\varepsilon) + \sum_{\alpha=0}^n (-1)^\alpha A_\alpha \left[\Delta_\varepsilon^\alpha u_\varepsilon - \Delta^\alpha u - \Delta_\varepsilon^\alpha u_\varepsilon + \Delta_\varepsilon^\alpha u \right] \right\} \\ &= \int_{\mathcal{C}} dx (\dot{u} - \dot{u}_\varepsilon) \left\{ u - u_\varepsilon + \sum_{\alpha=0}^n (-1)^\alpha A_\alpha (\Delta_\varepsilon^\alpha u - \Delta^\alpha u) \right\}. \end{aligned} \quad (3.48)$$

In the second step we have integrated by parts α times, in the third we have used the equations of motion. The last step follows by canceling two equal terms with opposite sign.

Hence the linear case goes exactly as in previous subsection, because $|\Delta_\varepsilon^\alpha u - \Delta^\alpha u| \leq \omega_\varepsilon$ for $\alpha \leq n$ and $u \in C^{2n+1}(\mathcal{C})$.

We summarize the results for the linear case in the following

Theorem 3.3. *Assume $R = 0$ and suppose that u_0 and v_0 satisfy (3.36). Let $u(t)$ be the classical solution to (3.37) and $u_\varepsilon(t)$ be the step function defined by (3.6) with $u_i(t)$, $i = 1, \dots, N$, solutions to (3.45) with initial data $u_i(0) = u_0(i\varepsilon)$ and $\dot{u}_i(0) = v_0(i\varepsilon)$.*

Then, for any $t \in [0, T]$,

$$\|u(t) - u_\varepsilon(t)\|_\varepsilon \rightarrow 0, \quad \text{as } \varepsilon \rightarrow 0,$$

where $\|\cdot\|_\varepsilon$ is the ε -dependent norm defined by

$$\|u\|_\varepsilon^2 = \int_C dx \left\{ |\dot{u}|^2 + |u|^2 + \sum_{k=1}^n |D_\varepsilon^k u|^2 \right\}. \quad (3.49)$$

Next we consider the nonlinear case. Now the equations of motion are (3.37) and (3.42) for the continuous and discrete system respectively. Defining W_ε by (3.47), by the same computation, we have, again using the summation by parts formula,

$$\begin{aligned} \frac{d}{dt} W_\varepsilon &= \int_C dx (\dot{u} - \dot{u}_\varepsilon) \left\{ (u - u_\varepsilon + \ddot{u} - \ddot{u}_\varepsilon) + \sum_{\alpha=0}^n A_\alpha D_\varepsilon^\alpha (\dot{u} - \dot{u}_\varepsilon) (D_\varepsilon^\alpha (u - u_\varepsilon)) \right\} \\ &= \int_C dx (\dot{u} - \dot{u}_\varepsilon) \left\{ (u - u_\varepsilon + \ddot{u} - \ddot{u}_\varepsilon) + \sum_{\alpha=0}^n (-1)^\alpha A_\alpha \Delta_\varepsilon^\alpha (u - u_\varepsilon) \right\} \\ &= \int_C dx (\dot{u} - \dot{u}_\varepsilon) \left\{ (u - u_\varepsilon) + \sum_{\alpha=0}^n (-1)^\alpha A_\alpha \left[\Delta_\varepsilon^\alpha u_\varepsilon - \Delta^\alpha u - \Delta_\varepsilon^\alpha u_\varepsilon + \Delta_\varepsilon^\alpha u \right] \right. \\ &\quad \left. + \left[-\partial_{\xi_0} R(u, Du) + D\partial_{\xi_1} R(u, Du) + \partial_{\xi_0} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon) - D_\varepsilon^- \partial_{\xi_1} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon) \right] \right\} \\ &= \int_C dx (\dot{u} - \dot{u}_\varepsilon) \left\{ u - u_\varepsilon + \sum_{\alpha=0}^n (-1)^\alpha A_\alpha (\Delta_\varepsilon^\alpha u - \Delta^\alpha u) \right. \\ &\quad \left. + \left[-\partial_{\xi_0} R(u, Du) + D\partial_{\xi_1} R(u, Du) + \partial_{\xi_0} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon) - D_\varepsilon^- \partial_{\xi_1} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon) \right] \right\} \end{aligned} \quad (3.50)$$

To control the non-linear terms we proceed by estimating:

$$T_1 = \partial_{\xi_0} R(u, Du) - \partial_{\xi_0} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon) = T_1^1 + T_1^2 \quad (3.51)$$

and

$$T_2 = D_\varepsilon^- [\partial_{\xi_1} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon)] - D[\partial_{\xi_1} R(u, Du)] = T_2^1 + T_2^2 \quad (3.52)$$

where

$$T_1^1 = \partial_{\xi_0} R(u, Du) - \partial_{\xi_0} R(u, D_\varepsilon^+ u), \quad (3.53)$$

$$T_1^2 = \partial_{\xi_0} R(u, D_\varepsilon^+ u) - \partial_{\xi_0} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon), \quad (3.54)$$

$$T_2^1 = D_\varepsilon^- [\partial_{\xi_1} R(u, D_\varepsilon^+ u)] - D[\partial_{\xi_1} R(u, Du)], \quad (3.55)$$

and

$$T_2^2 = D_\varepsilon^- [\partial_{\xi_1} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon)] - D_\varepsilon^- [\partial_{\xi_1} R(u, D_\varepsilon^+ u)]. \quad (3.56)$$

The bound (3.39) and Poincaré inequality imply that the L^∞ norms of u , Du and $D_\varepsilon^\pm u$ are bounded uniformly in ε . Thus, by the local Lipschitz continuity of $\partial_{\xi_0} R$, we have

$$|T_1^1| \leq C |Du - D_\varepsilon^+ u| \leq \omega_\varepsilon,$$

by the regularity of u . Thus, by the energy bounds (3.39) and (3.44) we get

$$\left| \int_C dx (\dot{u} - \dot{u}_\varepsilon) T_1^1 \right| \leq C [\mathcal{E}(u(0)) + \mathcal{E}_\varepsilon(u_\varepsilon(0))]^{\frac{1}{2}} \omega_\varepsilon,$$

To control T_1^2 we need L^∞ bounds for u_ε and $D_\varepsilon u_\varepsilon$. They follow from the conservation of the energy for the discrete system by means of the following

Lemma 3.4. *Let f be a step function on \mathcal{C} left continuous in the points $i\varepsilon$. Suppose that*

$$\|f\|_{H_\varepsilon^1}^2 = \int_{\mathcal{C}} dx(|f|^2 + |D_\varepsilon^+ f|^2)$$

is bounded. Then

$$\|f\|_\infty \leq C\|f\|_{H_\varepsilon^1}.$$

Proof. Let $x_0 = i_0\varepsilon$ be any point such that $|f(x_0)|^2 \leq \frac{1}{|\mathcal{C}|} \int_{\mathcal{C}} dx|f|^2$. Note that such a point does exist otherwise we would obtain a contradiction ($\int_{\mathcal{C}} dx|f|^2 > \int_{\mathcal{C}} dx|f|^2$). For $x = (i_0 + k)\varepsilon$ we have

$$f^2(x) = f^2(x_0) + \sum_{h=0}^{k-1} [f^2(x_0 + (h+1)\varepsilon) - f^2(x_0 + h\varepsilon)].$$

Since

$$\begin{aligned} |f^2(x + \varepsilon) - f^2(x)| &= |[f(x + \varepsilon) + f(x)][f(x + \varepsilon) - f(x)]| = \varepsilon[f(x + \varepsilon) + f(x)]D_\varepsilon^+ f| \\ &\leq \frac{1}{2}\varepsilon[f(x + \varepsilon) + f(x)]^2 + \frac{1}{2}\varepsilon|D_\varepsilon^+ f|^2, \end{aligned}$$

we conclude that

$$|f^2(x)| \leq \left(\frac{1}{|\mathcal{C}|} + 1\right) \int_{\mathcal{C}} dx|f|^2 + \frac{1}{2} \int_{\mathcal{C}} dx|D_\varepsilon^+ f|^2 \leq \left(\frac{1}{|\mathcal{C}|} + 1\right) \|f\|_{H_\varepsilon^1}^2.$$

□

Lemma 3.4 and the energy bound (3.44) imply that the L^∞ norms of u_ε and $D_\varepsilon^+ u_\varepsilon$ are bounded uniformly in ε . Thus we can use the Lipschitz continuity of $\partial_{\xi_0} R$ to get:

$$\left| \int_{\mathcal{C}} dx(\dot{u} - \dot{u}_\varepsilon)T_1^2 \right| \leq KW_\varepsilon,$$

with K the Lipschitz constant of $\partial_{\xi_0} R$ in the ball of radius $\max\{\|u\|_\infty, \|Du\|_\infty, \|u_\varepsilon\|_\infty, \|D_\varepsilon u_\varepsilon\|_\infty\}$.

The bound of T_2 , involving discrete derivatives, requires the following chain rule formula for the discrete derivative of a composite function:

Lemma 3.5. *If f has continuous first derivative f' , then for any function g and for any x there exist $\lambda_{\varepsilon,x} \in (0, 1)$ such that*

$$D_\varepsilon^\pm f(g(x)) = f'(\zeta_\varepsilon(x))D_\varepsilon^\pm g(x), \quad \text{with } \zeta_\varepsilon(x) = g(x) + \varepsilon\lambda_{\varepsilon,x}D_\varepsilon^\pm g(x)$$

Proof. By the mean value theorem, for D_ε^+ we have

$$D_\varepsilon^+ f(g(x)) = \varepsilon^{-1}[f(g(x + \varepsilon)) - f(g(x))] = \varepsilon^{-1} \int_{g(x)}^{g(x+\varepsilon)} dz f'(z) = \varepsilon^{-1}[g(x + \varepsilon) - g(x)]f'(\zeta)$$

for a suitable ζ in the interval with extremes $g(x)$ and $g(x + \varepsilon)$: $\zeta = g(x) + \lambda_{\varepsilon,x}[g(x + \varepsilon) - g(x)] = g(x) + \varepsilon\lambda_{\varepsilon,x}D_\varepsilon^+ g(x)$ for some $\lambda_{\varepsilon,x} \in (0, 1)$. In the same way the statement for D_ε^- follows. □

By the chain rule,

$$T_2^1 = \partial_{\xi_0, \xi_1}^2 R(\zeta_\varepsilon(x), D_\varepsilon^+ u)D_\varepsilon^- u - \partial_{\xi_0, \xi_1}^2 R(u, Du)Du + \partial_{\xi_1^2}^2 R(u, \eta_\varepsilon(x))\Delta_\varepsilon u - \partial_{\xi_1}^2 R(u, Du)\Delta u,$$

where

$$\zeta_\varepsilon(x) = u(x) + \varepsilon \lambda_{\varepsilon,x} D_\varepsilon^- u(x)$$

and

$$\eta_\varepsilon(x) = D_\varepsilon u(x) + \varepsilon \mu_{\varepsilon,x} \Delta_\varepsilon u(x),$$

with $\lambda_{\varepsilon,x} \in (0, 1)$, $\mu_{\varepsilon,x} \in (0, 1)$. But

$$\begin{aligned} \partial_{\xi_0, \xi_1}^2 R(\zeta_\varepsilon(x), D_\varepsilon^+ u) D_\varepsilon^- u - \partial_{\xi_0, \xi_1}^2 R(u, Du) Du = \\ \partial_{\xi_0, \xi_1}^2 R(u, Du) [D_\varepsilon^- u - Du] + D_\varepsilon^- u [\partial_{\xi_0, \xi_1}^2 R(\zeta_\varepsilon(x), D_\varepsilon^+ u) - \partial_{\xi_0, \xi_1}^2 R(u, Du)]. \end{aligned}$$

The smoothness of u and $D_\varepsilon u$ and the Lipschitz continuity of $\partial_{\xi_0, \xi_1}^2 R$ yield

$$|\partial_{\xi_0, \xi_1}^2 R(\zeta_\varepsilon(x), D_\varepsilon^+ u) - \partial_{\xi_0, \xi_1}^2 R(u, Du)| \leq C |D_\varepsilon^+ u - Du| \leq \omega_\varepsilon,$$

so also this term goes to 0 by the regularity of u .

Similarly,

$$\begin{aligned} \partial_{\xi_1}^2 R(u, \eta_\varepsilon(x)) \Delta_\varepsilon u - \partial_{\xi_1}^2 R(u, Du) \Delta u \\ = \partial_{\xi_1}^2 R(u, Du) [\Delta_\varepsilon u - \Delta u] + [\partial_{\xi_1}^2 R(u, \eta_\varepsilon(x)) - \partial_{\xi_1}^2 R(u, Du)] \Delta_\varepsilon u \end{aligned}$$

The first part goes to 0 by the regularity of u . By the boundedness of u , Du , $D_\varepsilon^\pm u$ and $\Delta_\varepsilon u$, we can use the Lipschitz continuity of $\partial_{\xi_1}^2 R$ to get the bound

$$|\partial_{\xi_1}^2 R(u(x), \eta_\varepsilon(x)) - \partial_{\xi_1}^2 R(u(x), Du(x))| \leq K |\eta_\varepsilon(x) - Du(x)|.$$

Since $\eta_\varepsilon(x) - Du(x) = D_\varepsilon^+ u(x) - Du(x) + \varepsilon \mu_{\varepsilon,x} \Delta_\varepsilon u(x)$,

$$|\eta_\varepsilon(x) - Du(x)| \leq |D_\varepsilon^+ u(x) - Du(x)| + \varepsilon \mu_{\varepsilon,x} |\Delta_\varepsilon u(x)|,$$

and hence

$$|\partial_{\xi_1}^2 R(u(x), \eta_\varepsilon(x)) - \partial_{\xi_1}^2 R(u(x), Du(x))| |\Delta_\varepsilon u(x)| \leq (|D_\varepsilon^+ u(x) - Du(x)| + \varepsilon \mu_{\varepsilon,x} |\Delta_\varepsilon u(x)|) |\Delta_\varepsilon u(x)|$$

But

$$|\Delta_\varepsilon u(x)| \leq |(\Delta_\varepsilon - \Delta)u(x)| + |\Delta u(x)|.$$

By the propagation of the initial regularity, $\|\Delta u(\cdot, t)\|_\infty$ is bounded for any $t \in (0, T)$. Therefore

$$|\partial_{\xi_1}^2 R(u(x), \eta_\varepsilon(x)) \Delta_\varepsilon u(x) - \partial_{\xi_1}^2 R(u(x), Du(x)) \Delta_\varepsilon u(x)| \leq \omega_\varepsilon.$$

As for the term T_2^2 , we use again the chain rule:

$$\begin{aligned} T_2^2 = D_\varepsilon^- [\partial_{\xi_1} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon)] - D_\varepsilon^- [\partial_{\xi_1} R(u, D_\varepsilon^+ u)] = \\ \partial_{\xi_0, \xi_1}^2 R(\zeta_\varepsilon(x), D_\varepsilon^+ u_\varepsilon) D_\varepsilon^- u_\varepsilon - \partial_{\xi_0, \xi_1}^2 R(\tilde{\zeta}_\varepsilon(x), D_\varepsilon^+ u) D_\varepsilon^- u + \partial_{\xi_1}^2 R(u_\varepsilon, \eta_\varepsilon(x)) \Delta_\varepsilon u_\varepsilon - \partial_{\xi_1}^2 R(u, \tilde{\eta}_\varepsilon(x)) \Delta_\varepsilon u, \end{aligned}$$

where

$$\begin{aligned} \zeta_\varepsilon(x) = u_\varepsilon(x) + \varepsilon \lambda_{\varepsilon,x} D_\varepsilon^- u_\varepsilon(x), \quad \tilde{\zeta}_\varepsilon(x) = u(x) + \varepsilon \lambda_{\varepsilon,x} D_\varepsilon^- u(x) \\ \eta_\varepsilon(x) = D_\varepsilon^+ u_\varepsilon(x) + \varepsilon \mu_{\varepsilon,x} \Delta_\varepsilon u_\varepsilon(x), \quad \tilde{\eta}_\varepsilon(x) = D_\varepsilon^+ u(x) + \varepsilon \mu_{\varepsilon,x} \Delta_\varepsilon u(x). \end{aligned}$$

We use the energy bound and Lemma 3.4 to get the boundedness of ζ_ε and $D_\varepsilon^\pm u_\varepsilon$ and thus the Lipschitz continuity of $\partial_{\xi_0, \xi_1}^2 R$, so that

$$\begin{aligned} & |\partial_{\xi_0, \xi_1}^2 R(\zeta_\varepsilon, D_\varepsilon^+ u_\varepsilon) D_\varepsilon^- u_\varepsilon - \partial_{\xi_0, \xi_1}^2 R(\tilde{\zeta}_\varepsilon, D_\varepsilon^+ u) D_\varepsilon^- u| \\ & \leq |\partial_{\xi_0, \xi_1}^2 R(\tilde{\zeta}_\varepsilon, D_\varepsilon^+ u)| |D_\varepsilon^- u_\varepsilon - D_\varepsilon^- u| + K |D_\varepsilon^- u_\varepsilon| |\zeta_\varepsilon(x) - \tilde{\zeta}_\varepsilon(x)|. \end{aligned}$$

But

$$|\zeta_\varepsilon(x) - \tilde{\zeta}_\varepsilon(x)| = |u_\varepsilon(x) - u(x)| + \varepsilon(|D_\varepsilon^- u_\varepsilon| + |D_\varepsilon^- u|),$$

so that

$$\int_C |dx| |\dot{u} - \dot{u}_\varepsilon| |D_\varepsilon^+ [\partial_{\xi_1} R(u_\varepsilon, D_\varepsilon^+ u_\varepsilon)] - D_\varepsilon [\partial_{\xi_1} R(u, D_\varepsilon^+ u)]| \leq C W_\varepsilon + \frac{1}{2} \varepsilon^2 (\mathcal{E}[u(0)] + \mathcal{E}_\varepsilon[u_\varepsilon(0)])$$

The term $\partial_{\xi_1}^2 R(u_\varepsilon, \eta_\varepsilon(x)) \Delta_\varepsilon u_\varepsilon - \partial_{\xi_1}^2 R(u, \tilde{\eta}_\varepsilon(x)) \Delta_\varepsilon u$ is more delicate because, in order to use Lipschitz continuity, we need to bound $\eta_\varepsilon(x)$ and hence the supremum of $\Delta_\varepsilon u_\varepsilon$. But Lemma 3.4 and energy conservation are not enough when $n = 2$. However we need really to bound $\varepsilon \Delta_\varepsilon u_\varepsilon$ and we can take advantage of this extra ε . Indeed, by the energy conservation and the positivity assumptions on R and A ,

$$\varepsilon A_{n,n}(D_\varepsilon^n u_\varepsilon(x))^2 \leq C,$$

and hence

$$|D_\varepsilon^n u_\varepsilon| \leq \frac{C}{\sqrt{\varepsilon}}, \quad (3.57)$$

implying that $|\eta_{\varepsilon,x}| \leq C$ (if $n > 2$ we get a better estimate). Thus we have

$$\begin{aligned} & |\partial_1^2 R(u_\varepsilon, \eta_\varepsilon) \Delta_\varepsilon u_\varepsilon - \partial_1^2 R(u, \tilde{\eta}_\varepsilon) \Delta_\varepsilon u| \leq |\partial_{\xi_1}^2 R(u, \tilde{\eta}_\varepsilon(x))| |\Delta_\varepsilon u - \Delta_\varepsilon u_\varepsilon| \\ & + |\partial_{\xi_1}^2 R(u, \tilde{\eta}_\varepsilon(x)) - \partial_{\xi_1}^2 R(u, \eta_\varepsilon(x))| |\Delta_\varepsilon u_\varepsilon| + |\partial_{\xi_1}^2 R(u_\varepsilon, \eta_\varepsilon(x)) - \partial_{\xi_1}^2 R(u, \eta_\varepsilon(x))| |\Delta_\varepsilon u_\varepsilon|. \end{aligned}$$

But, by (3.57),

$$|\eta_\varepsilon(x) - \tilde{\eta}_\varepsilon(x)| = |D_\varepsilon^-(u_\varepsilon(x) - u(x))| + \varepsilon(|\Delta_\varepsilon u_\varepsilon| + |\Delta_\varepsilon u|) \leq \omega_\varepsilon.$$

Therefore, by the Cauchy-Schwartz inequality and conservation of energy, we obtain that

$$\int_C |dx| |\dot{u} - \dot{u}_\varepsilon| |\partial_{\xi_1}^2 R(u_\varepsilon, \eta_\varepsilon) \Delta_\varepsilon u_\varepsilon - \partial_{\xi_1}^2 R(u, \tilde{\eta}_\varepsilon) \Delta_\varepsilon u| \leq C W + \omega_\varepsilon.$$

Collecting all the terms, we conclude that there is a constant $C > 0$ such that

$$\frac{d}{dt} W_\varepsilon \leq C W_\varepsilon + \omega_\varepsilon,$$

and hence, by Gronwall lemma

$$|W_\varepsilon(t)| \leq |W_\varepsilon(0)| e^{Ct} + t e^{Ct} \omega_\varepsilon \quad \text{as } \varepsilon \rightarrow 0.$$

We summarize the results in the following

Theorem 3.6. *Suppose that u_0 and v_0 satisfy (3.36). Let $u(t)$ be the solution to (3.37) and $u_\varepsilon(t)$ be the step function defined by (3.6) with $u_i(t)$, $i = 1, \dots, N$, solutions to (3.45) with initial data $u_i(0) = u_0(i\varepsilon)$ and $\dot{u}_i(0) = v_0(i\varepsilon)$. Then for any $t > 0$,*

$$\|u(t) - u_\varepsilon(t)\| \rightarrow 0, \quad \text{as } \varepsilon \rightarrow 0,$$

in the norm defined in (3.49).

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